Counting crystal momentum (k) values

G.-H. Gweon, Phys 155, Winter 2008, UCSC

1 Basic fact

For a given crystal with N primitive unit cells, there are N distinct crystal momentum values.

This statement is generally applicable to any waves in crystal, phonons, electrons, or any other waves. For the electron case, an equivalent statement [which is the basis for Wilson's rule] is that, to fill an electron band dispersion completely, we need 2 electrons per unit cell, considering the additional spin degeneracy.

2 Proof

As usual, we work with the periodic boundary (Born von Karman) condition [not essential, but strongly recommended for all discussions of physics of bulk]. Take a three dimensional crystal with primitive lattice given by $\vec{a}, \vec{b}, \vec{c}$, which, in general, do not have to be orthogonal to each other and do not have to have the same length either. We view our crystal as being in the form of [in general] a parallel pipe formed by three vectors $N_1\vec{a}$, $N_2\vec{b}$, $N_3\vec{c}$. So, the total number of unit cells in our crystal is $N_1N_2N_3$. We can define this to be N [obviously this definition depends on dimensions, see below]. The periodic boundary condition means that we join end faces (resulting in "hyper-torus" which is impossible to visualize!), and the allowed $\vec{k}$ values are given by $\frac{l\vec{a}^*}{N_1}$, $\frac{m\vec{b}^*}{N_2}$, $\frac{n\vec{c}^*}{N_3}$, where l, m, n are integers. I emphasize that these allowed values are the results of the boundary condition [think plane waves that are periodic with periods $N_1\vec{a}$, $N_2\vec{b}$, $N_3\vec{c}$].

1. Note that per each $\vec{k}$ value, a volume $v^* = \frac{|(\vec{a}^* \times \vec{b}^*) \cdot \vec{c}^*|}{N_1N_2N_3} = \frac{|(\vec{a}^* \times \vec{b}^*) \cdot \vec{c}^*|}{N}$ can be assigned. (In a cubic crystal $v^* = \frac{(2\pi)^3}{a^3N} = \frac{(2\pi)^3}{L^3}$, assuming the crystal is a cube with dimensions $L \times L \times L$.) Often I described v^* as "quantum" of $\vec{k}$ in class.

2. **Any given volume V in $\vec{k}$ space contains $\frac{V}{v^*}$ crystal momentum values.**

3. For a unit cell in $\vec{k}$ space, the volume is given by $V_{unit} = |(\vec{a}^* \times \vec{b}^*) \cdot \vec{c}^*|$, and thus the above "bacic fact" is proven by dividing V_{unit} by v^*.

4. Note that this proof can be immediately generalized to any dimensions, if we replace "volume" with "hyper-volume," change the definition of N, and replace $(\vec{a}^* \times \vec{b}^*) \cdot \vec{c}^*$ with a more appropriate expression for the given dimension. To be specific:

   (a) In one dimension: hyper-volume=length, $N = N_1$, $v^* = \frac{|a^*|}{N_1} = \frac{2\pi}{Na} = \frac{2\pi}{L}$, $V_{unit} = |a^*| = \frac{2\pi}{a}$.

   (b) In two dimensions: hyper-volume=area, $N = N_1N_2$, $v^* = \frac{|\vec{a}^* \times \vec{b}^*|}{N_1N_2} = \frac{|\vec{a}^* \times \vec{b}^*|}{N}$, $V_{unit} = |\vec{a}^* \times \vec{b}^*|$.